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UNCLASSIFIED TR-23 NL

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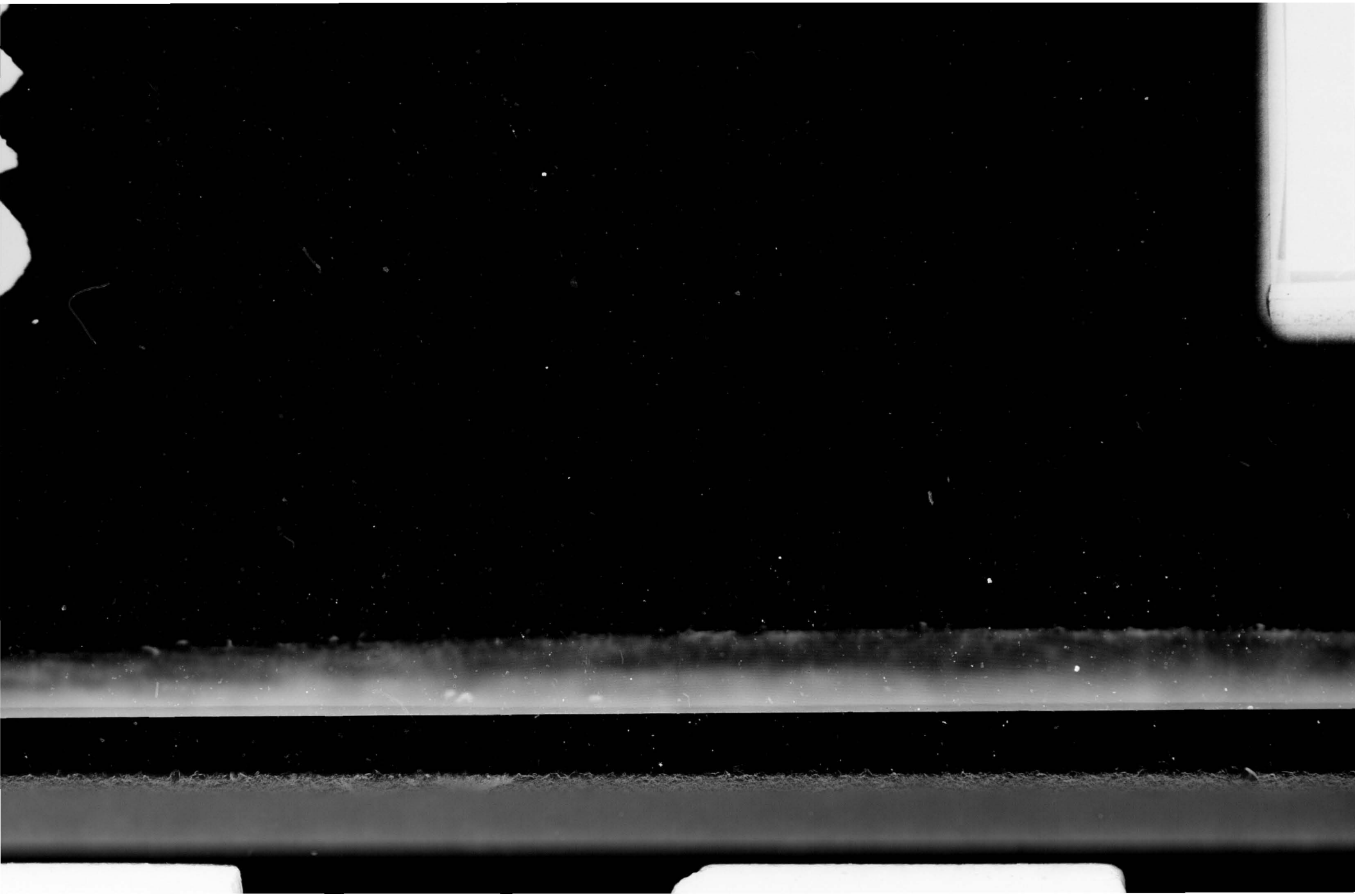

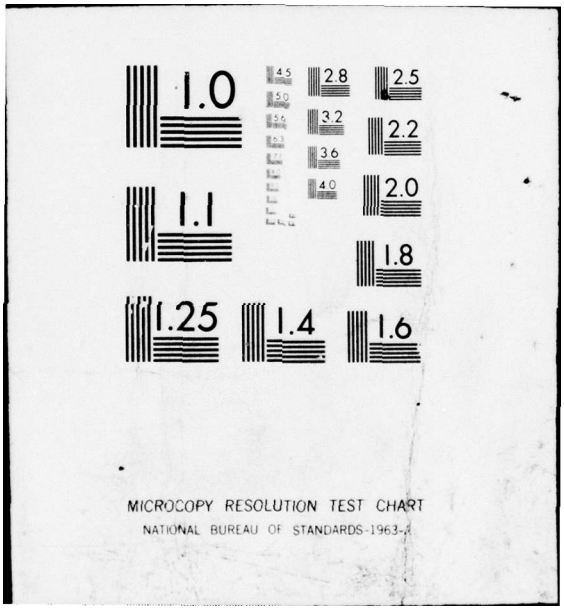
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by

M.F. McCarthy and H.F. Tiersten

Office of Naval Research
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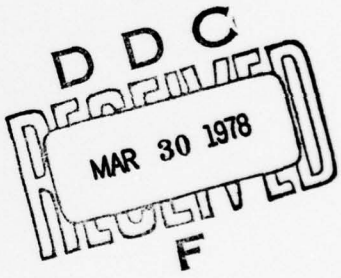

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Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: No. 23 (14) TR-23
2. GOVT ACCESSION NO.
3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle): (6) ON INTEGRAL FORMS OF THE BALANCE LAWS FOR DEFORMABLE SEMICONDUCTORS

5. TYPE OF REPORT & PERIOD COVERED: (9) Technical Report
6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s): (10) M.F. McCarthy and H.F. Tiersten

8. CONTRACT OR GRANT NUMBER(s): (15) N0014-76-C-0368, NSF-ENG72-04223

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Department of Mechanical Engineering,
Aeronautical Engineering & Mechanics
Rensselaer Polytechnic Institute
Troy, New York 12181

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
NR 318-009

11. CONTROLLING OFFICE NAME AND ADDRESS
Office of Naval Research
Physics Branch
Washington, D.C. 20360

12. REPORT DATE: (11) Feb 78

13. NUMBER OF PAGES: 15 (12) 19 p.

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)

15. SECURITY CLASS. (of this report): Unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Distribution of this document is unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Deformable Semiconductors	Semiconduction	Continuum Physics
Balance Laws	Electroelasticity	Thermodynamics
Integral Forms	Elasticity	
Electrical Conduction	Jump Conditions	
Heat Conduction	Nonlinear Interactions	

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

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ON INTEGRAL FORMS OF THE BALANCE LAWS FOR DEFORMABLE SEMICONDUCTORS

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ABSTRACT

The general nonlinear differential equations describing the interaction of finitely deformable, polarizable, heat conducting intrinsic n-type semiconductors with the quasi-static electric field are transformed from the unknown present coordinate description to the known reference coordinate description, which is the form needed in the treatment of problems. From the differential form of each balance equation in the reference coordinate description, the associated integral form is obtained. The resulting integral forms turn out as expected with the exception of the one due to the balance of linear momentum for the semiconducting fluid, in which an important change in and simplification from the form used heretofore is introduced. More importantly, the previous existing integral form of the equation of the balance of energy in the present coordinate description is transformed to a different form, which is equivalent to the original form only when the field variables are differentiable. The revised integral form in the present coordinate description is then transformed to the reference coordinate description, from which an energetic jump condition across a moving non-material surface of discontinuity is obtained which is consistent with all the other jump conditions obtained from the other integral forms. In addition, the expression for the quasi-static electric Poynting vector in the reference coordinate description is determined.

1. Introduction

In a treatment of the interaction of the quasi-static electric field with a finitely deformable, polarizable, heat conducting, dielectric continuum a system of rotationally invariant differential equations and jump conditions were derived[1]. First, the differential equations were obtained from a systematic application of the laws of continuum physics to a well-defined macroscopic model. Then, the integral forms obtained from the respective differential forms were taken to be valid across moving surfaces of discontinuity even when the differential forms from which they were obtained did not hold because of the lack of differentiability across the singular surface. This is a standard, perfectly reasonable procedure for obtaining the governing integral forms for an interacting continuum. The jump conditions across moving, not necessarily material, surfaces of discontinuity were then obtained from the respective integral forms. The resulting integral forms and associated jump conditions were referred to the unknown present (spatial) coordinates of material points whereas it would have been more useful to refer them to the known reference (material) coordinates of material points. However, this is not a severe limitation since it is a straight-forward matter to transform from present to reference coordinates of material points using well known relations. Nevertheless, although in the work[1] in question the appropriate reference forms of the jump conditions for the balance of mass, linear momentum, charge and entropy may readily be obtained in the aforementioned manner, the reference form of the jump condition for the balance of energy may not be obtained directly from the equations presented in Ref.1. Indeed, although the integral form of the equation of the balance of energy is not incorrect, the present form of the jump condition for the balance of energy presented there[1] is not directly useful for application to problems concerning

the propagation of surfaces of discontinuity and, hence, is not actually correct. This dilemma is a consequence of the fact that the integral form of the balance of energy is not unique because the differential form can have terms added to it which vanish at each volumetric point and yet give surface terms. Since the field variables are not differentiable when the jump conditions are obtained from the integral forms, the different integral forms yield different jump conditions which are not equivalent. In a later work[2] the treatment was extended from the case of deformable insulators[1] to deformable semiconductors. In the latter work[2] although an integral form of the equation of the conservation of energy is written, the associated jump condition is not because the authors were aware of the problem involved.

In this paper the proper revised differential form of the equation of the conservation of energy is found for the more general case of the deformable semiconductor. From the revised differential form the appropriate integral form of the equation of the conservation of energy is obtained in both the present and reference coordinate descriptions, from which the required correct energetic jump condition in the reference coordinate description is obtained. One by-product of this work is the determination of the proper expression for the quasi-static Poynting vector in the reference coordinate description. In addition to the foregoing a new integral form of the equation of the conservation of linear momentum for the free-electronic charge continuum is introduced. The new form is better for obtaining jump conditions because certain assumptions that had to be made in obtaining jump conditions from the previous form[2,3] need not be made with the present form. Moreover, the jump condition at a material surface of discontinuity resulting from the present form will be different from and more convincing than the one obtained from the previous form.

2. Basic Equations

It has been shown[2] that a system of general nonlinear rotationally invariant differential equations for deformable intrinsic n-type semiconductors can be written in the form[3]

$$(\tau^{S}_{ij} + T^{ES}_{ij} - p^{e}\delta_{ij})_{,i} = \rho\, dv_j/dt\,, \tag{2.1}$$

$$\partial\mu/\partial t + j_{i,i} = 0\,,\quad D_{i,i} = \mu\,, \tag{2.2}$$

$$E^{e}_{i} = (\varphi + \varphi^{e})_{,i}\,,\quad E_i = -\varphi_{,i}\,, \tag{2.3}$$

$$j_i = \mu v_i + \mu^{e}(v^{e}_{i} - v_i)\,,\quad \mu = \mu^{e} + \mu^{r}\,, \tag{2.4}$$

$$T^{ES}_{ij} = \epsilon_o E_i E_j - \frac{1}{2}\epsilon_o E_k E_k \delta_{ij}\,, \tag{2.5}$$

$$-\mu^{e} E^{e}_{i}(v^{e}_{i} - v_i) - q_{i,i} = \rho\theta\, d\eta/dt\,, \tag{2.6}$$

where τ^{S}_{ij} and T^{ES}_{ij} denote the symmetric parts of the usual mechanical and free-space Maxwell electrostatic stress tensors, respectively; v^{e}_{i}, v_j, E^{e}_{i}, E_i, D_i, j_i and q_j denote the velocity of the free electronic fluid, velocity of the solid, local material electric field exerted on the free electronic fluid, Maxwell electric field, electric displacement, electric current and heat flux vector, respectively; μ^{e}, p^{e}, ρ, φ, φ^{e}, μ, μ^{r}, θ and η denote the free electronic charge density, free electronic pressure, mass density, electric potential, free electronic chemical potential, net charge density, residual lattice charge density, temperature and entropy per unit mass, respectively; and ϵ_o is the permittivity of free space. The motion of a point of the solid is described by the mapping

$$y_i = y_i(X_L, t)\,, \tag{2.7}$$

where y_i denotes the present coordinates of material points and X_L, the reference coordinates, and t denotes the time. Clearly, we have

$$v_i = \partial y_i/\partial t . \tag{2.8}$$

In (2.1) - (2.8) we have used Cartesian tensor notation, the summation convention for repeated tensor indices, the convention that a comma followed by an index denotes partial differentiation with respect to a coordinate, and the convention that capital indices refer to reference coordinates and lower case indices to present coordinates of material points.

The associated constitutive equations take the form

$$\tau^S_{ij} = \rho y_{i,K} y_{j,L} \frac{\partial \chi}{\partial E_{KL}} , \quad D_i = \epsilon_o E_i - \rho y_{i,L} \frac{\partial \chi}{\partial W_L} , \tag{2.9}$$

$$v^e_i - v_i = y_{i,K} \Omega^e_K , \quad \eta = - \partial \chi/\partial \theta , \quad q_i = y_{i,K} L_K , \tag{2.10}$$

$$p^e = (\mu^e)^2 \partial \epsilon^e/\partial \mu^e , \quad \varphi^e = \partial(\mu^e \epsilon^e)/\partial \mu^e , \tag{2.11}$$

where

$$\chi = \chi(E_{KL}, W_L, \theta) , \quad \Omega^e_K = \Omega^e_K(\mu^e, w^e_L, E_{KL}, W_L, \theta) ,$$

$$\epsilon^e = \epsilon^e(\mu^e) , \quad L_K = L_K(\theta_{,M}, \mu^e, w^e_L, E_{LM}, W_L, \theta) , \tag{2.12}$$

and

$$E_{KL} = \frac{1}{2} (y_{i,K} y_{i,L} - \delta_{KL}) , \quad W_L = y_{i,L} E_i , w^e_L = y_{i,L} E^e_i . \tag{2.13}$$

In addition, we have the conservation of mass, which may be written in the form

$$\rho J = \rho_o , \tag{2.14}$$

where ρ_o is the reference mass density and

$$J = \det y_{i,K} . \tag{2.15}$$

At this point we note that the above system of equations is referred to the present coordinates, which are unknown, and, as a consequence, it is advantageous to refer them to the known reference coordinates. To this end, analogous to the Piola-Kirchhoff stress tensor F_{Lj}, which is defined by

$$n_i T_{ij}\, dS = N_L F_{Lj}\, dS_o , \tag{2.16}$$

we define the reference electric displacement vector $\mathcal{D}_L$ by[4,5]

$$n_i D_i\, dS = N_L \mathcal{D}_L\, dS_o , \tag{2.17}$$

where dS_o and N_L denote the magnitude of and unit normal to an element of area in the reference configuration, which has magnitude dS and unit normal n_i in the present configuration. By virtue of the well-known relation[6]

$$n_i\, dS = JX_{L,i} N_L\, dS_o , \tag{2.18}$$

from (2.16) and (2.17), in the usual way, we find

$$F_{Lj} = JX_{L,i} T_{ij} , \quad \mathcal{D}_L = JX_{L,i} D_i . \tag{2.19}$$

By defining the reference free-space Maxwell electrostatic stress tensor M_{Lj} and free electronic pressure tensor $\mathcal{P}^e_{Lj}$ in a similar way we find

$$M_{Lj} = JX_{L,i} T^{ES}_{ij} , \quad \mathcal{P}^e_{Lj} = JX_{L,j} p^e . \tag{2.20}$$

Now, using (2.19) and (2.20) with (2.1) and $(2.2)_2$ and employing (2.14) along with the well-known identity[7]

$$(JX_{L,i})_{,L} = 0 , \tag{2.21}$$

we obtain

$$(F_{Lj} + M_{Lj} - \mathcal{P}^e_{Lj})_{,L} = \rho_o dv_j/dt , \tag{2.22}$$

$$\mathcal{D}_{L,L} = \bar{\mu} , \tag{2.23}$$

where

$$\bar{\mu} = J\mu . \tag{2.24}$$

Equation (2.22) is the Piola-Kirchhoff form of the stress equations of motion for the combined deformable semiconducting continuum and Eq. (2.23) is the

reference form of the charge equation of electrostatics. From (2.3), the chain rule of differentiation and $(2.13)_3$, we obtain

$$w^e_L = (\varphi + \varphi^e)_{,L} \tag{2.25}$$

which is the reference form of the equation of the conservation of linear momentum for the free electronic charge continuum.

In order to refer the conservation of total electric charge to the known reference configuration X_L instead of the unknown present configuration y_i to which it is referred in $(2.2)_1$, we write

$$j'_i = j_i - \mu v_i , \tag{2.26}$$

the substitution of which in $(2.2)_1$ along with the aid of (2.24) and the well-known relations

$$d/dt = (\partial/\partial t) + v_k \partial/\partial y_k , \quad v_{k,k} = J^{-1} dJ/dt , \tag{2.27}$$

yields

$$j'_{i,i} + J^{-1} d\bar{\mu}/dt = 0 . \tag{2.28}$$

Now, we define the reference electric current vector $\mathcal{J}_L$ by

$$n_i j'_i dS = N_L \mathcal{J}_L dS_o , \tag{2.29}$$

which with (2.18) yields

$$\mathcal{J}_L = J X_{L,i} j'_i , \tag{2.30}$$

from which with (2.28) and (2.21) we obtain

$$\mathcal{J}_{L,L} + d\bar{\mu}/dt = 0 , \tag{2.31}$$

which is the reference form of the conservation of total electric charge.

Analogous to the foregoing, we now define the reference heat flux vector Q_L by

$$n_i q_i \, dS = N_L Q_L \, dS_o , \tag{2.32}$$

which with (2.18) yields

$$Q_L = J X_{L,i} q_i . \tag{2.33}$$

Substituting from $(2.10)_1$, (2.13) and (2.33) into (2.6) and employing (2.14) and (2.21) we obtain

$$-\bar{\mu}^e w_K^e \Omega_K^e - Q_{L,L} = \rho_o \theta \, d\eta/dt , \tag{2.34}$$

where

$$\bar{\mu}^e = J\mu^e . \tag{2.35}$$

Equation (2.34) is the reference form of the dissipation equation. The associated reference form of the Clausius-Duhem inequality takes the form

$$\rho_o \frac{d\eta}{dt} + \left(\frac{Q_L}{\theta}\right)_{,L} = -\frac{1}{\theta}\left[\frac{Q_L \theta_{,L}}{\theta} + \bar{\mu}^e w_L^e \Omega_L^e\right] = \rho_o \Gamma \geq 0 , \tag{2.36}$$

where Γ is the (positive) rate of entropy production.

From $(2.4)_1$, (2.9), (2.10), (2.19), (2.26), (2.30), (2.33) and (2.35) the pertinent constitutive equations can be written in the form

$$F_{Lj} = \rho_o y_{j,M} \frac{\partial \chi}{\partial E_{LM}} , \quad \mathcal{S}_L = \epsilon_o \mathcal{E}_L - \rho_o \frac{\partial \chi}{\partial W_L} , \tag{2.37}$$

$$\mathcal{J}_L = \bar{\mu}^e \Omega_L^e , \quad Q_K = J L_K , \tag{2.38}$$

where

$$\mathcal{E}_L = J X_{L,i} E_i , \tag{2.39}$$

and the constitutive equations in (2.11) and $(2.10)_2$ remain unchanged along with the expressions for χ, Ω_K^e, ϵ^e and L_K in (2.12) and, of course, (2.5) and (2.20) are to be employed. From $(2.3)_2$ and $(2.13)_2$ we note that

$$W_K = -\varphi_{,K}.$$

The integral forms of Eqs. (2.22), (2.23), (2.25), (2.31) and (

referred to the known reference coordinates of material points, whi

prime interest to us here, clearly may be written

$$\int_{S_o} N_L (F_{Lj} + M_{Lj} - \mathscr{P}^e_{Lj}) dS_o = \frac{d}{dt} \int_{V_o} \rho_o v_j \, dV_o ,$$

$$\int_{S_o} N_L \mathscr{P}_L \, dS_o = \int_{V_o} \bar{\mu} \, dV_o ,$$

$$\int_{V_o} w^e_L \, dV_o = \int_{S_o} N_L (\varphi + \varphi^e) \, dS_o ,$$

$$\int_{S_o} N_L \mathscr{J}_L \, dS_o = - \frac{d}{dt} \int_{V_o} \bar{\mu} dV_o ,$$

$$\frac{d}{dt} \int_{V_o} \rho_o \eta \, dV_o + \int_{S_o} \frac{N_L Q_L}{\theta} \, dS_o = - \int_{V_o} \frac{1}{\theta} \left[\frac{Q_L \theta_{,L}}{\theta} + \mathscr{J}_L w^e_L \right] dV_o \geq 0 .$$

The integral form in (2.43) is different than the equivalent equati

has been employed heretofore[2,3,8]. Equation (2.43) is a better for

obtaining the jump condition for the free-electronic charge continu

both material and nonmaterial surfaces of discontinuity. Since Eq.

does not contain the free electronic charge density μ^e explicitly,

assumption on the boundedness of μ^e need be made in obtaining jump

and, as a consequence, the resulting jump conditions are independen

Maxwell tensor and the associated assumptions that have been used p

From the integral forms in (2.41) - (2.45), jump conditions across m

necessarily material surfaces of discontinuity can readily be obtai

suitable assumptions. For example, at a nonmaterial surface of dis

we assume that all volumetric density terms remain bounded and in the usual way obtain

$$N_{L\sim}[\mathscr{A}_{Lj\sim}] = -\,U_N \rho_{o\sim}[v_{j\sim}]\,,\quad N_{L\sim}[\mathscr{B}_{L\sim}] = 0\,,\quad \underset{\sim}{[\varphi + \varphi^e]} = 0\,, \tag{2.46}$$

$$N_{L\sim}[\mathscr{E}_{L\sim}] = U_{N\sim}[\bar{\mu}]\,,\quad N_{L\sim}[Q_L/\theta] - U_N \rho_{o\sim}[\eta] \geq 0\,, \tag{2.47}$$

where U_N is the intrinsic[9] velocity of the singular surface, we have introduced the conventional notation $\underset{\sim}{[a]}$ for $a^- - a^+$ and

$$\mathscr{A}_{Lj} = F_{Lj} + M_{Lj} - \mathscr{P}^e_{Lj}\,. \tag{2.48}$$

Since E_i remains bounded, we have

$$\underset{\sim}{[\varphi]} = 0\,, \tag{2.49}$$

and, hence, from $(2.46)_3$ we obtain

$$\underset{\sim}{[\varphi^e]} = 0\,. \tag{2.50}$$

The integral form of the equation of the conservation of energy and associated jump condition has not been discussed here because the existing integral form has to be revised in accordance with the detailed discussion presented in the next section.

3. Integral Form of the Balance of Energy

In this section we consider the equation of the conservation of energy for the deformable intrinsic n-type semiconductor, the integral form of which may be written

$$\frac{d}{dt}\int_V \left[\frac{1}{2}\,\rho v_k v_k + \rho\varepsilon + \mu^e \varepsilon^e + \frac{1}{2}\,\epsilon_o E_k E_k\right] dV = \int_S n_i \Big[\bar{\tau}_{ij} v_j - p^e v_i^e - h_i - q_i - (v_i^e - v_i)\mu^e \varepsilon^e + v_i P_k E_k + v_i\,\frac{1}{2}\,\epsilon_o E_k E_k\Big]\, dS\,, \tag{3.1}$$

where P_k denotes the electric polarization per unit volume and for the quasi-static electric field[10]

$$h_i = \varphi[(\partial D_i/\partial t) + j_i] , \tag{3.2}$$

in MKS units. Equation (3.1) is the extension of Eq. (5.4) of Ref.1 for the deformable insulator to the deformable intrinsic n-type semiconductor and is also Eq. (4.14) of Ref.2 when reduced to the special case of the intrinsic n-type semiconductor in a quasi-static electric field. Since the total stress tensor S_{ij} appears in the equation of the conservation of linear momentum for the combined continuum, i.e., (2.1), (2.22) and (2.41), we write

$$S_{ij} = \tau_{ij} + T^E_{ij} - p^e\delta_{ij} , \tag{3.3}$$

where

$$T^E_{ij} = \left[D_iE_j - \frac{1}{2}\epsilon_o E_k E_k \delta_{ij}\right], \quad \tau_{ij} = \tau^S_{ij} - P_iE_j ; \tag{3.4}$$

and since

$$D_i = \epsilon_o E_i + P_i . \tag{3.5}$$

from (3.3) - (3.5) and (2.5) we note that in addition

$$S_{ij} = \tau^S_{ij} + T^{ES}_{ij} - p^e\delta_{ij} . \tag{3.6}$$

We now substitute from (3.3) with $(3.4)_1$, $(2.4)_1$, (2.11), (2.26), (3.2) and (3.5) into (3.1) to obtain

$$\frac{d}{dt}\int_V \left[\frac{1}{2}\rho v_k v_k + \rho\varepsilon + \mu^e\varepsilon^e + \frac{1}{2}\epsilon_o E_k E_k\right] dV = \int_S n_i\Big[S_{ij}v_j - D_iE_jv_j + E_jD_jv_i - \varphi^e j_i' - \varphi\frac{\partial D_i}{\partial t} - \varphi j_i - q_i\Big] dS . \tag{3.7}$$

Now, consider the term

$$\int_S n_i[E_jD_jv_i - D_iE_jv_j]\, dS = t , \tag{3.8}$$

the application of the divergence theorem to which yields

$$t = \int_V [E_jD_jv_i - D_iE_jv_j]_{,i}\, dV . \tag{3.9}$$

Moreover, appropriate differentiation and the substitution of $(2.3)_2$ enables the integrand in (3.9) to be written

$$(E_j D_j v_i - D_i E_j v_j)_{,i} = - [\varphi (D_j v_i - D_i v_j)_{,i}]_{,j}, \tag{3.10}$$

since

$$(D_j v_i - D_i v_j)_{,ij} = 0. \tag{3.11}$$

Substituting from (3.10) into (3.9), employing the divergence theorem and $(2.2)_2$, we obtain

$$t = - \int_S n_i \varphi (D_{i,j} v_j + D_i v_{j,j} - D_j v_{i,j} - \mu v_i) dS, \tag{3.12}$$

the substitution of which into (3.7) yields

$$\frac{d}{dt} \int_V \left[\frac{1}{2} \rho v_k v_k + \rho \varepsilon + \mu^e \varepsilon^e + \frac{1}{2} \varepsilon_o E_k E_k \right] dV = \int_S n_i \Big[S_{ij} v_j - \varphi \Big(D_{i,j} v_j + D_i v_{j,j} - D_j v_{i,j} - \mu v_i + \frac{\partial D_i}{\partial t} + j_i \Big) - \varphi^e j_i' - q_i \Big] dS, \tag{3.13}$$

in place of (3.7). Equation (3.13) is another integral form of the equation of the balance of energy referred to present coordinates, which is entirely equivalent to (3.7) when the field variables are differentiable. However, when the field variables are not differentiable, the two integral forms obviously are not equivalent.

Equation (3.13) is the appropriate form for obtaining the energetic jump condition in the reference coordinate description while Eq. (3.7) is not. To see this note that the material time derivative of the reference electric displacement vector $\mathcal{D}_L$ defined in $(2.19)_2$ may be written

$$\frac{d}{dt} \mathcal{D}_L = J X_{L,i} \Big[\frac{\partial D_i}{\partial t} + v_j D_{i,j} - D_j v_{i,j} + v_{j,j} D_i \Big], \tag{3.14}$$

where $(2.7)_2$ and the well-known relation

$$(d/dt) X_{K,j} = - X_{K,i} v_{i,j}, \tag{3.15}$$

have been employed in obtaining (3.14) from $(2.19)_2$. Now, substituting from (3.14), (3.6), (2.14), (2.16), (2.18), (2.20), (2.26), (2.29), (2.32), (2.35) and (2.48) into (3.13), we obtain

$$\frac{d}{dt}\int_{V_o}\left[\frac{1}{2}\rho_o v_k v_k + \rho_o \varepsilon + \overline{\mu}^e \varepsilon^e + \frac{1}{2}\varepsilon_o E_k E_k J\right] dV_o = \int_{S_o} N_L\left[\mathscr{A}_{Lj} v_j - \varphi\left(\frac{d}{dt}\mathscr{D}_L + \mathscr{J}_L\right) - \varphi^e \mathscr{J}_L - \mathscr{Q}_L\right] dS_o , \tag{3.16}$$

which is the integral form of the balance of energy in the reference coordinate description we have been after. An examination of (3.16) reveals that the quasi-static electric Poynting vector referred to the known reference coordinates takes the form

$$h_L = \varphi\left(\frac{d}{dt}\mathscr{D}_L + \mathscr{J}_L\right), \tag{3.17}$$

in MKS units. The energetic jump condition across moving non-material surfaces of discontinuity may readily be obtained from (3.16) by assuming that all volumetric density terms remain bounded with the result

$$N_L\left[\mathscr{A}_{Lj} v_j - h_L - \varphi^e \mathscr{J}_L - \mathscr{Q}_L\right] = - U_N \rho_o [\Omega] , \tag{3.18}$$

where h_L is given in (3.17) and

$$\Omega = \frac{1}{2} v_k v_k + \varepsilon + \frac{\mu^e \varepsilon^e}{\rho} + \frac{1}{2}\frac{\varepsilon_o}{\rho} E_k E_k . \tag{3.19}$$

It should be noted that the jump condition in (3.18) is consistent with all the other jump conditions appearing in Sec.2, while the jump condition obtained from (3.1) [or (3.7)] would be inconsistent with the jump condition in $(2.46)_1$ in most cases.

Acknowledgements

This work was supported in part by the Office of Naval Research under Contract No. N00014-76-C-0368 and the National Science Foundation under Grant No. ENG 72-04223.

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